Virtual Design and Testing of Materials: A Multiscale Approach

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14. ABSTRACT
The aim of this work proposed here is the development of a virtual testing and design capability that can be used to test, and suggest design strategies for, new advanced structured materials.

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2. Objectives

The aim of the work proposed here is the development of a virtual testing and design capability that can be used to test, and suggest design strategies for, new advanced structural materials. Our main objective is thus to develop a hierarchy of methods involving both seamless coupling of information from different scales (electronic to atomic; atomic to microstructural; micro- to macrostructural) and information transfer from one level of hierarchy to the next. As a secondary objective, each methodological advance will also be used to investigate specific phenomena at a single scale. The general plan is shown schematically in Figure 1. The overall outcome of our work will be a coherent set of computational tools and advances in fundamental understanding of many issues in the thermomechanical performance of materials.

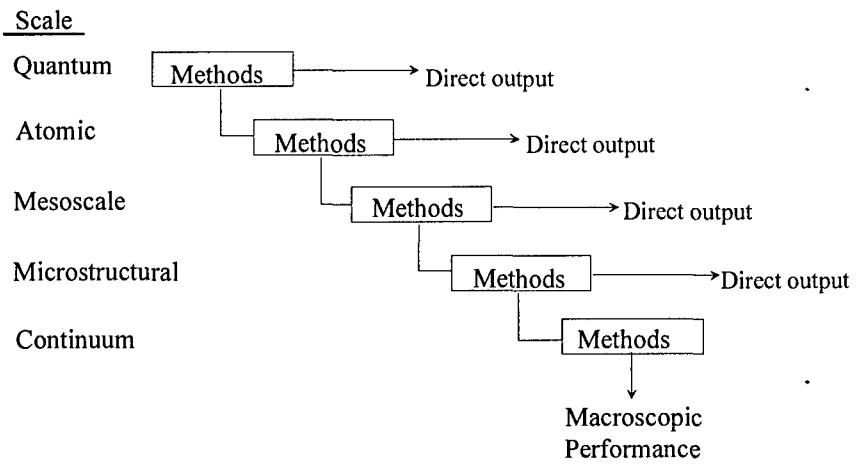

Figure 1. Schematic of direct output at each scale, and use of output at one scale as input to next higher scale.

Within the broad objectives above, our major specific technical objectives are:

(1) develop new methods to couple highly accurate quantum chemical methods and Density Functional Theories (DFT) for electronic structure in real space for extended systems, which will permit the study of atom energetics in highly heterogeneously strained environments (surfaces, cracks, dislocations);

(2) develop new models based on the quasicontinuum method (QC) to incorporate the direct quantum mechanical methods and finite temperatures from (1) and formulate a coupled Kinetic-Monte-Carlo/QC/Continuum-diffusion approach to simulating corrosion reactions at the nanoscale;

(3) utilize the new QC models to analyze dislocation structure, mobility, and interactions at finite temperatures; to predict cracking and deformation at metal/metal-oxide interfaces; and to examine fundamental impurity and dislocation interactions relevant to hardening;

(4) establish methods to incorporate atomistic information on dislocation nucleation, motion, and interactions into mesoscale discrete-dislocation simulation models, and simulate the formation of fatigue damage at crack tips and boundaries, including environmentally-assisted fatigue;

(5) incorporate atomistic information into new cohesive zone models for describing deformation and failure at metal/metal-oxide interfaces and under fatigue and corrosion conditions;
(6) combine discrete dislocation models and new cohesive zone models, both informed from explicit atomistic features, into single crystal plasticity simulation models; simulate the static and fatigue performance of textured polycrystals using this approach, including consideration of the stochastic effects of microstructure.

As a demonstration of these capabilities, and to provide specific focus to the overall research, we aim to predict the nano-, micro-, and macroscopic degradation of Aluminum and Titanium alloys under fatigue loading and in a corrosive (oxidative) environment and as a function of temperature.

3. Status of Effort

The program has now ended and all funds have been expended. A final review was held at AFOSR on November 2, 2006 to brief the program manager and other DOD and government agency personnel on the accomplishments of the program. This report summarizes some main accomplishments of the program against the program objectives.

4. Accomplishments

This MURI program can claim a number of "firsts" in the field of multiscale modeling as a result of our research to achieve the program objectives. In this final report, we briefly discuss the most important of these "firsts".

1. First model predicting fatigue crack growth behavior with no a priori assumptions about fatigue (Discrete Dislocation Model)

The discrete dislocation model developed by Needleman and co-workers approaches plastic deformation by dealing directly with the physics and mechanics at the individual dislocation level. The material behavior introduced into the calculation thus involves only dislocation nucleation, motion, annihilation, and interactions, all of which are independent of the particular problem being investigated. The system response under a particular mode of testing is governed by the evolution of the dislocation system in response to the boundary conditions of the desired test. In this MURI, the discrete dislocation method has been shown to predict fatigue crack growth from pre-existing cracks with no fatigue-specific input. Rather, in the presence of an initial crack and under cyclic macroscopic applied loading, the dislocation system organizes into a structure that toughens the material against fracture but also that drives fracture forward. Fatigue features are thus entirely an output of the computation. Work in this MURI has shown that this model predicts the following features observed in many experiments: (i) a threshold value of loading for the onset of fatigue crack growth; (ii) a cross-over to a power-law regime of crack growth rate versus applied loading (Paris-law behavior), (iii) a dependence of the threshold on local reversibility of the fracture process, attributable to oxidation or other fracture surface chemical reactions, (iv) acceleration or deceleration of the crack growth rate due to single-cycle overloading of the system, (v) accelerated crack

growth at small crack sizes and other so-called "short crack" effects, (vi) an independence of the fatigue threshold and the material yield strength; (vii) fatigue "striations" on the crack surface. This physics-based approach to plastic deformation is now serving as a test bed to probe other problems in fatigue crack growth (thin films; bimaterials; growth around cracked inclusions) and to predict the salient physical features in a variety of small-scale plasticity phenomena.

2. First method for combining continuum and atomistic descriptions of defects within one framework.

Curtin and coworkers developed the "Coupled Atomistic/Discrete-Dislocation" (CADD) model that combines the power of the discrete dislocation model with the atomistic resolution of molecular dynamics. At the atomistic scale, the model builds on the Quasicontinuum idea but uses a modified atom/continuum coupling method that eliminates spurious forces and an efficient and accurate approach for studying finite temperature dynamics in the atomistic region. Most importantly, dislocation defects can exist in either the atomistic domain, as dislocations with a fully-resolved atomistic core, and as continuum discrete dislocation entities, and such dislocations can move from one description to the other as dictated by the forces driving dislocations and the overall plasticity. The ability, in CADD, to model non-trivial deformation behavior, i.e. the motion of dislocations, in the continuum region is unique to date.

The method has now been applied to a number of demonstration problems such as indentation and simple fracture. In addition, it has been applied to the complex problem of dislocation/grain-boundary interactions, which can control Hall-Petch behavior and/or be the source of damage accumulation and nucleation in polycrystalline metals. A current application is to hydrogen embrittlement in Iron.

3. First model to couple of quantum mechanics and atomistic models for metals.

Kaxiras and coworkers have developed a new method to embed quantum mechanical calculations, using either standard density functional theory (DFT) or orbital-free DFT (OF-DFT), within an atomistic computational model that employs semi-empirical atomistic potentials. Such a quantum/atomistic coupling of metals is far more difficult than coupling in covalently bonded materials because of the highly delocalized nature of the metallic electrons. The coupling method is built upon a creative decoupling of the total energies in the overall problem, leading to a quantum computation on a region of material that is influenced by the electron density provided by the surrounding semi-empirical atoms in the material. The problem of charge accumulation at the boundaries, due to a mismatch in material descriptions, has been greatly reduced through the use of corrective forces derived from the model. The method has been applied to study dislocation-dislocation interactions in Aluminum, and to study dislocation nucleation from a crack tip in Aluminum.

3. A finite-temperature Quasicontinuum model;

Phillips and coworkers have extended the original static, zero-temperature Quasicontinuum model to finite temperatures. The approach starts by considering a formal "coarse graining" of the microscopic partition function of a classical material at finite temperature. An approximate effective coarse-grained potential is then generated

by making a self-consistent quasi-harmonic approximation for the atoms that have been eliminated through the coarse-graining process. This self-consistent procedure accounts for the entropy that can be lost in coarse-graining and addresses the dependence of the free energy on the mechanical deformation state of the material. These two features are essential in capturing the proper finite-temperature material behavior. The resulting model, which includes a correction for the extra entropy that is introduced in the finite element nodes and addresses the appropriate methods for dealing with the mass of the nodes, predicts the thermal expansion and finite-T elastic constants in very good agreement with full molecular dynamics simulations of the same problem up to fairly high temperatures. Using this finite-T QC model, the full thermodynamics of a coupled atomistic/continuum system is computed automatically with no inputs other than the atomic interactions and the crystal structure. The model has been applied to a simple indentation problem to demonstrate the effects of finite temperature on the load required to nucleate a dislocation underneath a cylindrical indenter.

4. First quantum/continuum coupling method.

Carter and Ortiz have developed the framework and code to utilize first-principles OF-DFT calculations into the "local" Quasicontinuum model. The QC uses the energy of strained unit cells of material to compute the deformation in continuum domains treated using finite-elements. Use of the OF-DFT method is crucial here because of the very large number of computations required to solve for the complex deformation state in a large-scale structure. The method has been applied to compare the predictions for nucleation of dislocations underneath an indenter as predicted by using the full quantum input and by using the typical semi-empirical potential input. Notable differences emerge, showing that the non-linear features of the deformation are important and that quantum-based calculations of highly-deformed material are likely necessary to properly model the true physics of any particular problem.

5. First quantum-mechanical determination of decohesion with and without impurity embrittlement.

Ceder, Carter, and coworkers have used quantum-mechanical methods (DFT) to predict the fundamental cohesive behavior of metals with and without H and O impurities along the separating surfaces. Ceder developed the appropriate thermodynamic potential, the so-called Grand Force potential, for converting computational result on decohesion at fixed impurity concentration to decohesion at fixed chemical potential, since the latter is appropriate in most physical situations. Ceder showed that the cohesive strength of Aluminum drops precipitously, from ~12GPa to 4GPa (in H) and 1-2 GPa (in O), when the chemical potential exceeds a critical value. Therefore, if impurity-driven crack growth occurs under quasi-equilibrium conditions, a severe embrittlement can be expected above the critical chemical potential. Carter computed decohesion energies in the Fe-H system and the Al-H system, demonstrating how the Born-Haber cycle can be used to compute proper surface energies. Carter also elucidated the differences between material separation in metals and oxides due to the differences in very local bonding character as material planes separate.

6. New methodology for informed continuum model of cracking by chemical embrittlement

Ortiz and Carter used the first-principles decohesion results of Carter and Ceder to develop a continuum simulation of stress-corrosion cracking in steels. An integral part of the modeling was the renormalization of the first-principles decohesion, occurring at length scales of an Angstrom, into an effective cohesion law at a length scale suitable for efficient continuum modeling. The model also included the stress-dependent diffusion of chemical species (e.g. H) through the material in the presence of the non-uniform crack tip field. The resulting simulation shows that the crack jumps in spurts: H accumulates at the crack tip and decreases the cohesion over some length ahead of the crack tip; at a critical concentration, the crack advances rapidly forward through the embrittled region; diffusion then occurs while the crack is arrested at the new position. Ortiz and coworkers applied the model to steels, and made predictions of the average crack velocity versus applied load and material yield strength that agree quite well with available experimental data. A number of features observed experimentally are predicted, such as a threshold load for crack growth, a power-law regime, the length of spurts in the crack growth, and an initial incubation time at the start of the test. The overall methodology thus demonstrates how first-principals input can be profitably used to properly inform a large-scale continuum simulation of a complex problem.

7. First basic discrete/continuum model for non-steady state flow of diffusing species.

Curtin and coworkers made further basic progress in bridging time scales for material transport. Specifically, they developed an approach for handling multiscale diffusion wherein one region of material is treated using full discreteness of the diffusing entities while another, much larger, region is treated using the continuum diffusion equation. By making the discrete region small, considerable time is saved in computations, permitting much longer simulations with no loss in accuracy. The method uses a domain-decomposition approach typical for solving partial-differential equations but adapted here to handle one domain in which the behavior is actually discrete. At the continuum/discrete interface, the method ensures flux continuity (essential for conserving mass of the species) and enforces concentration continuity on an average basis. Application to simple demonstration problems shows that the method agrees perfectly, within natural statistical fluctuations, with a fully-discrete model of the same simple problem, thus showing that the discrete/continuum interface is handled without introduction of any artifacts.

Summary

We have accomplished nearly all of the original goals of the program (those established upon proposal or as refined within the first year of the program). Above, we highlighted a handful of "firsts" in the field of multiscale modeling, and discussed only briefly the specific applications. These highlights do not reflect the entire scope of the research performed, which is captured in the many publications (see below). Recognition of the research success in this program and the leadership of the investigators in the field of multiscale modeling can be seen through the many invited talks (over 135 during the program) and published papers (over 85 published during the program), a number of which are seminal review articles. Furthermore, a number of the accomplishments within

this program are now finding interest and application from a spectrum of industrial laboratories. Thus, theoretical developments in this program are proving to be immediately useful to major industrial users/developers of advanced materials in the US. We believe that this MURI program has provided the Department of Defense agencies with a significant portfolio of multiscale research tools that will serve to accelerate the evaluation and testing of advanced materials and systems in the years to come.

5. Personnel Supported

Details of personnel supported can be found in the yearly reports.

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7. Interactions/Transitions

a. Invited Talks

Over 125 invited talks at national and international venues. A complete listing can be compiled from prior reports on this project.

b. Consultative/Advisory

c. Transitions:

A number of graduate students received PhD degrees during the course of this program:

Dr. S. Curatolo received a PhD from MIT and won the Materials Research Society (MRS) Graduate Student Award (2002).
Dr. Robin L. Hayes received a PhD from UCLA 2004, winning the Dissertation Award for the Best Physical Chemistry Dissertation at UCLA.
Dr. Baojing Zhou received a PhD from UCLA in 2004.
Dr. De-en Jiang received a PhD from UCLA in 2005.
Dr. Michael O'day received a PhD from Brown in 2004.
Dr. Michael Dewald received a PhD from Brown in 2006.
Dr. Matt Fago received a PhD from Cal Tech in 2004.
Dr. Emily Jarvis received a PhD from UCLA in 2002.
Dr. Nick Choly received a PhD in Physics from Harvard in 2004.

Several post-doctoral associates and students who worked on the program have now moved into academic positions at major US universities, forming a core of next-

generation scientists and engineers knowledgable in multiscale modeling in mechanics and materials:

Dr. Amine Benzerga, Assistant Professor at Texas A&M
Dr. Anton van der Ven, Assistant Professor at U. Michigan
Dr. Gang Lu, Assistant Professor at Cal State Northridge
Dr. S. Curatolo, Assistant Professor at Duke

8. New Discoveries, inventions, patents None

9. Honors/Awards:

Faculty involved in the MURI received a number of honors and awards, including:

E. A. Carter was named to the Marks Endowed Chair in Mechanical Engineering at Princeton University

M. Ortiz was named the Dotty and Dick Hayman Professor of Aeronautics and Mechanical Engineering at Cal Tech.

W. A. Curtin was named the Elisha Benjamin Andrews Professor at Brown University.

W. A. Curtin was awarded a Guggenheim Fellowship for 2005-2006 to pursue his research in the area of Multiscale Modeling of Materials.

W. A. Curtin was appointed Editor-in-Chief of Modeling and Simulation in Materials Science and Engineering in July 2005.

E. A. Carter was elected a Fellow of the Institute of Physics in 2004.

E. A. Carter was named the 2005 Merck-Frosst Lecturer at Concordia University.

A. Needleman won the Prager Medal from the Society of Engineering Science, 2005.

A. Needleman received an honorary doctorate from the Danish Technical University, 2006.

A. Needleman received an honorary doctorate from Ecole Normal Superieur du Cachan, France, 2006.

M. Ortiz received an award from the Alexander von Humboldt Foundation.

M. Ortiz received the Computational Mechanics Award from the International Association for Computational Mechanics.